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Measurement and Simulation of Herbicide Transport in Macroporous Soils

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Abstract: Lysimeter experiments were carried out to study pesticide transport through macroporous soils. In order to differentiate between the effects of soil structure and chemical behaviour, the leaching experiments were conducted using disturbed and undisturbed soil samples. Two herbicides with different sorption behaviours, and bromide as tracer were applied. The results were used to validate a dynamic simulation model which considers bypass flow in macropores. The simulation results show that the model is able to reproduce the soil suction within the soil as well as the spatial distribution of bromide and the herbicides. The continuity of the macropores is most important for the efficiency of bypass flow. The results indicate that cultivation practices like ploughing significantly influence the temporal and spatial distribution of the macropores. © 1998 SCI.

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Key words: herbicide leaching; macropores; bypass flow; lysimeter experiments; simulation model

1 INTRODUCTION

Groundwater is an important source of drinking water, supplying 75% or more of the drinking water in Germany. During recent years, contamination of groundwater by pesticides has generated environmental problems.

When pesticides reach the soil, they may undergo microbial and/or chemical degradation, photodecomposition, volatilisation, plant uptake and adsorption. Furthermore, losses can occur by surface run-off and leaching through the soil profile. Water that infiltrates through the soil may carry pesticides through and below the root zone, possibly reaching groundwater. Many pesticides with different physical-chemical properties have been found in groundwater.[1] In many cases the reasons for such contamination are not clear. In the past, the description of flow processes in the soil profile considered only matrix flow. However, the results of transport experiments can often not be explained solely by the convective-dispersive theory.[2,3] Only the presence of preferential pathways can explain fast vertical transport.

A number of field and laboratory studies have shown that preferential flow is an important mechanism in the movement of pollutants to groundwater.[2,4] Preferential flow can be defined as flow through macropores (i.e. earthworm and root channels, shrinking cracks), transport through zones with high conductivity[5] and fingering as a result of fluid instability. In particular, macropore flow takes place only in a small part of the soil[6] and can be initiated under a number of different conditions. The transport of water and pesticides is affected also by rainfall intensity.[7] Soil tillage is also an important factor for macropore flow. The phenomenon of macropore flow is summarised by Van Genuchten *et al.*[8]

In this study, soil column experiments were carried out to examine the transport of water, bromide and selected herbicides in a well-structured, water-unsaturated loess soil. The data were used for the validation of a simulation model.

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2 METHODS AND MATERIALS

The studies were carried out using small-scale lysimeters with loess soil (soil type: Gleyic Luvisol, silt loam). The soil was taken from an agricultural site (Neuenkirchen) located in Lower Saxony in the region of Braunschweig, Germany. Details of the investigated site are given by McVoy *et al.*[9] The most important soil parameters are shown in Table 1. It is a highly structured soil with continuous earthworm channels down to a depth of 1 m. Undisturbed soil samples were taken in soil column cylinders (diameter 0·30 m, length 0·85 m).

Five undisturbed (S1–S5) and one reference (S6) soil columns were investigated. The reference soil (S6) core was prepared by sieving (2 mm) and repacking the soil of a disturbed soil sample. The resulting bulk density in the subsoil (0·30–0·85 m) was slightly lower than that of the undisturbed soil cores (S6 = 1·34 g cm^{-3}, undisturbed soil mean 1·47 ($\pm$0·03) g cm^{-3}).

Soil sampling was carried out using hydraulic pressure equipment.[10] After screwing two anchors into the soil, they were connected with a horizontal anchor beam. The pressing of the cylinders into the soil was done by a hydraulic jack placed between the cylinder and the anchor beam.

After sampling, the soil monoliths were installed in the experimental set-up (Fig. 1). A sprinkling device was set on top of the column. It ensured a good spatial distribution of the irrigation water by supplying it from 89 hypodermic needles. The irrigation cycles were set by a time-limit relay which controlled a pump and a magnetic valve. This equipment allowed quasi-continuous watering at low flow rates.

The bottom of the soil column was installed on a special plate, the outlet from which ended in a low-pressure chamber. Permanent suction of −20 hPa was applied during all experiments to avoid soil water saturation in the lowest soil layer. A fraction collector was used to sample the percolating water. To prevent the intake of air into the soil column, an air-impermeable layer was put between soil and the plate. This microporous diaphragm acted in a way similar to a ceramic plate.

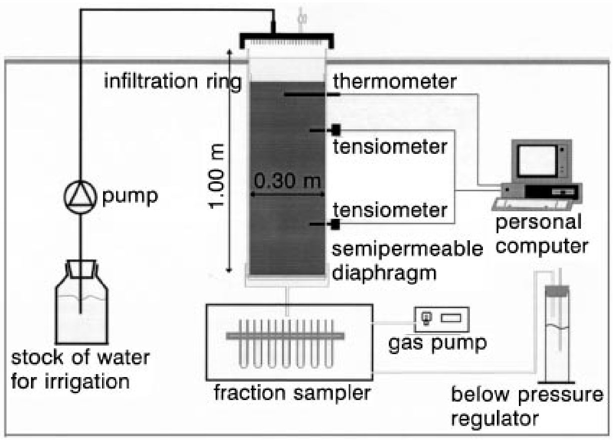

Fig. 1. Experimental set-up for testing leaching behaviour of herbicides in unsaturated, structured soil.

Tensiometers with electronic pressure transducers were installed horizontally (0·25 m and 0·75 m above the bottom). Measurements were made continuously and stored every two minutes on a personal computer (A/D interface card). The experiments were carried out in an air-conditioned chamber at controlled temperature from 7 to 14°C.

Three irrigations (60 min.) were applied with a 48-h interval between each. The rainfall intensity was 25 mm h^{-1}. This value represented the intensity of a heavy rainfall. The percolate collection was done at 36-min intervals. Before starting leaching experiments, all soil samples were irrigated (1 mm h^{-1} until outflow occurred) to ensure the same initial water content. After that, the lysimeters drained for two weeks to reach field capacity. Two herbicides, chlorotoluron (CT) and methabenzthiazuron (MBT), were applied at 10 kg ha^{-1} and 14 kg ha^{-1}. The solute was pipetted in a fine grid to give a good spatial distribution.

After the leaching experiments, the soil was removed from the bottom of the columns in 5-cm segments. Every 5 cm the occurrence of macropores (pores with a diameter >1 mm) was visually examined and transferred over a transparent foil. The macropores were divided into three classes (from 1 to 4 mm, from 4 to 8 mm and larger than 8 mm).

TABLE 1
Soil Characteristics

	Topsoil	*Subsoil*		
Soil depth (m)	0·00–0·30	0·30–0·50	0·50–0·75	0·75–0·85
Soil texture (%)				
Sand	2·1	3·7	2·7	1·9
Silt	78·8	70·4	78·7	82·1
Clay	19·1	25·7	18·6	16·0
pH value ($CaCl_2$)	6·9	7·1	7·5	7·5
Organic carbon (%)	1·3	0·5	0·3	0·2
Bulk density (g cm^{-3})	1·38	1·44 (0·30–0·85 m)		

TABLE 2
Estimated Parameters of the Water Retention Curve of Van Genuchten.[12] The standard deviations of these estimates are shown in brackets.

Sample	*O1*	*O2*	*O3*	*O4*	*O5*	*O6*	*Mean*	*Median*
θ_s ($cm^3\ cm^{-3}$)	41·256	45·583	46·701	44·718	50·501	46·449	45·868	46·016
	(0·652)	(0·836)	(0·617)	(1·288)	(2·199)	(0·831)		
α (hPa^{-1})	0·0064	0·0093	0·0146	0·0228	0·0450	0·0124	0·0184	0·0135
	(0·0019)	(0·0029)	(0·0030)	(0·0105)	(0·0287)	(0·0036)		
n (−)	1·243	1·242	1·227	1·196	1·181	1·230	1·220	1·229
	(0·027)	(0·029)	(0·017)	(0·029)	(0·034)	(0·025)		
R^2	0·9921	0·9913	0·9962	0·9841	0·9742	0·9928		
Sample	*U1*	*U2*	*U3*	*U4*	*U5*	*U6*	*Mean*	*Median*
θ_s ($cm^3\ cm^{-3}$)	44·445	43·296	41·596	42·055	41·136	43·840	42·728	42·676
	(0·454)	(0·602)	(0·740)	(0·637)	(0·787)	(1·215)		
α (hPa^{-1})	0·2229	0·0557	0·0325	0·0287	0·0328	0·0651	0·0730	0·0443
	(0·0326)	(0·0122)	(0·0098)	(0·0075)	(0·0109)	(0·0291)		
n (−)	1·134	1·155	1·164	1·167	1·158	1·144	1·154	1·157
	(0·004)	(0·009)	(0·014)	(0·127)	(0·015)	(0·016)		
R^2	0·9990	0·9970	0·9938	0·9953	0·9926	0·9885		

Herbicides were extracted and enriched from 10 ml percolate by using a Baker-10 Extraction System (C_{18}-solid phase extraction, SPE). After elution, they were analysed by high performance liquid chromatography (HPLC) with UV-detector. The quantification was done with regard to peak height and internal standard. The recovery rate for CT in the subsoil (0·30–0·85 m) as well as in the topsoil (0–0·30 m) was more than 110% for all four concentrations (see also Table 2). For MBT the recovery increased with concentration and also from the top to the subsoil in the range from 88 to 98%.

Additionally a tracer (bromide) was applied at 200 kg ha^{-1} with the irrigation water. In the first and the second columns (S1 and S2) 150 kg ha^{-1} bromide was applied. The bromide was analysed by ion exchange chromatography after filtering the water samples (membrane filter, 0·45 mm). In order to characterise the soil physical properties, six samples of the topsoil (O1–O6) and six samples of the subsoil (U1–U6) were taken from the field to measure retention curves in the laboratory. The results of the experiments were fitted to the retention function of Van Genuchten by means of the statistic program *Statgraphics*. The estimated values of the saturated moisture content θ_s and the empirical constants α and n are shown in Table 2.

The values of saturated hydraulic conductivity are in the range typical for a structured soil. The results are from 13·2 to 308·2 cm day^{-1} in the topsoil and 16·4 to 653·3 cm day^{-1} in the subsoil (Table 3). In many cases (e.g. Hartge and Horn[11]) it has been shown that the saturated conductivity follows log normal distribution. The mean of the logarithms of the saturated conductivity values was therefore used for the simulation (topsoil: 34·8 cm day^{-1}, subsoil: 65·1 cm day^{-1}). The unsaturated conductivity was derived from the estimated values for α and n according to the formula of Van Genuchten.[12]

3 SIMULATION MODEL

In this study, the model SIMULAT[13,14] was employed. SIMULAT is a system for simulating water and solute transport, soil temperature, dynamics of nitrogen and sulphur, and the dynamics of pesticides and their metabolites. For calculating the fate of pesticides, SIMULAT includes a model bank for degradation,

TABLE 3
Saturated Hydraulic Conductivity

Soil sample	*O1*	*O2*	*O3*	*O4*	*O5*	*O6*	*Log-mean*	*Median*
Conductivity (cm day^{-1})	18·9	308·2	78·0	20·7	14·3	13·2	34·8	19·8
Soil sample	*U1*	*U2*	*U3*	*U4*	*U5*	*U6*	*Log-mean*	*Median*
Conductivity (cm day^{-1})	167·0	30·4	653·3	61·1	16·4	22·8	65·1	45·8

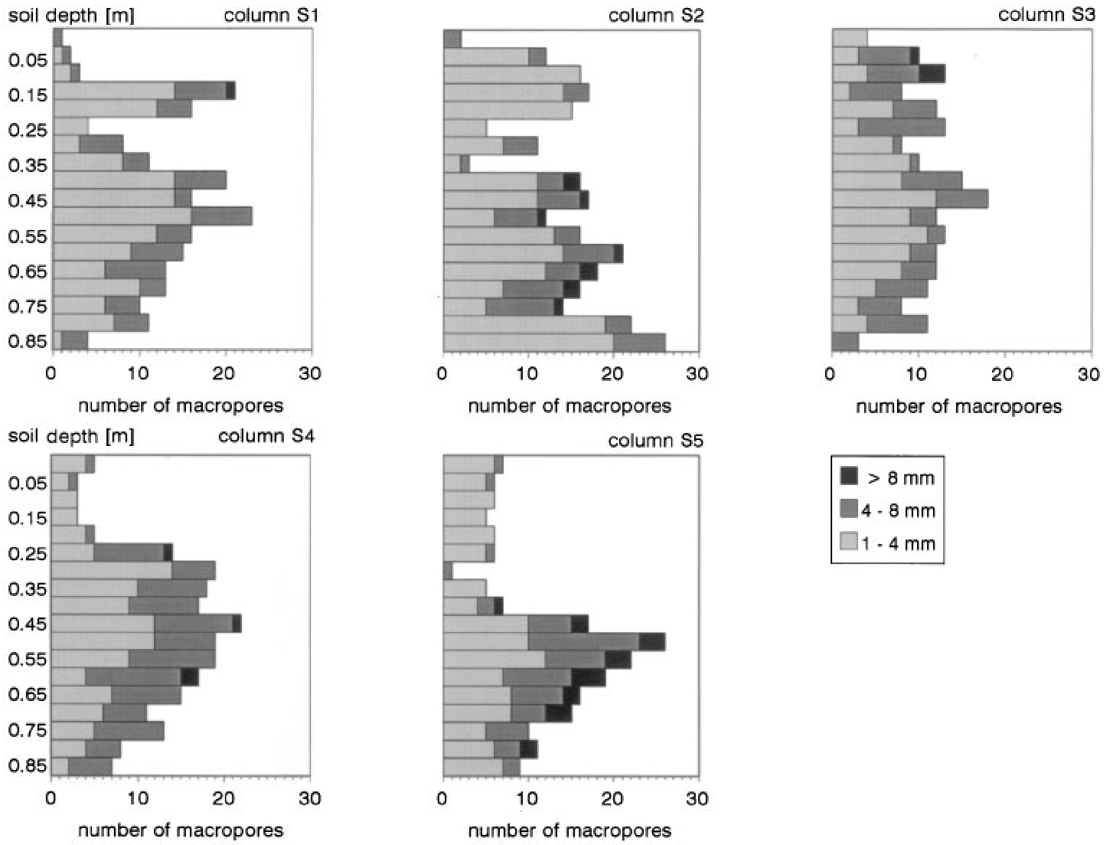

Fig. 2. Distribution and size of the macropores in the undisturbed soil columns S1–S5.

sorption and dependencies on environmental variables. It considers different sorption isotherms, biotic (metabolic and cometabolic) and abiotic degradation, and different approaches for calculating temperature and moisture dependencies. In addition to the one-dimensional water and solute transport, evapotranspiration, interception and plant growth is simulated. Because in this study only water and solute transport in structured porous media are investigated the model description given here is limited to these processes.

In the classical Richards' equation it is assumed that water transport in porous media can be described by a macroscopic approach. The relationship between soil tension and water content is often described by a unimodal pore-size distribution. This approach fails in all situations where microscopic structures like fractures, fissures, aggregate pores and macropores influence the water fluxes significantly, resulting in transport behaviour not explainable by the one-domain approach (preferential flow). Therefore, in the past, models for water transport in structured porous media have been developed which describe the water transport in a two-domain approach. While most of the models concentrate on matrix and macropore flow[15,16] only a few approaches assume two (or more) capillary flow domains.[17,18]

If macropores exist, the water flow cannot be described by the capillary two-domain concept. In this case Richards' equation for one-dimensional water flow in the soil matrix (mi)

$$\frac{\partial \theta_{\mathrm{mi}}}{\partial t} = \frac{\partial}{\partial z}\left(K_{\mathrm{mi}}(\psi_{\mathrm{mi}})\left(\frac{\partial \psi_{\mathrm{mi}}}{\partial z} - 1\right)\right) - S_{\mathrm{w}} \tag{1}$$

is coupled to the water flow in the macropore system (ma)

$$\frac{\partial \theta_{\mathrm{ma}}}{\partial t} = \frac{\partial q_{\mathrm{ma}}}{\partial z} + S_{\mathrm{w}} \tag{2}$$

by the exchange term S_{w}

$$S_{\mathrm{w}} = K_{\mathrm{lat}} \frac{\psi_{\mathrm{mi}} - \psi_{\mathrm{ma}}}{\Delta x} \tag{3}$$

in which θ is the water content, ψ the soil suction, $K = K(\psi)$ the unsaturated hydraulic conductivity, K_{lat} the lateral saturated hydraulic conductivity, t the time and z the vertical coordinate. Assuming film flow in the macropores ($\psi_{\mathrm{ma}} = 0$), Δx of eqn (3) is given as the half-width of the matrix pore system. According to Germann and Beven[15] the gravity flow of water in the macropores can be described by the following relationship between water flux, q_{ma}, and the macropore moisture content θ_{m}

$$q_{\mathrm{ma}} = K_{\mathrm{s\,ma}}\left(\frac{\theta_{\mathrm{ma}}}{\theta_{\mathrm{s\,ma}}}\right)^{a_{\mathrm{ma}}} \tag{4}$$

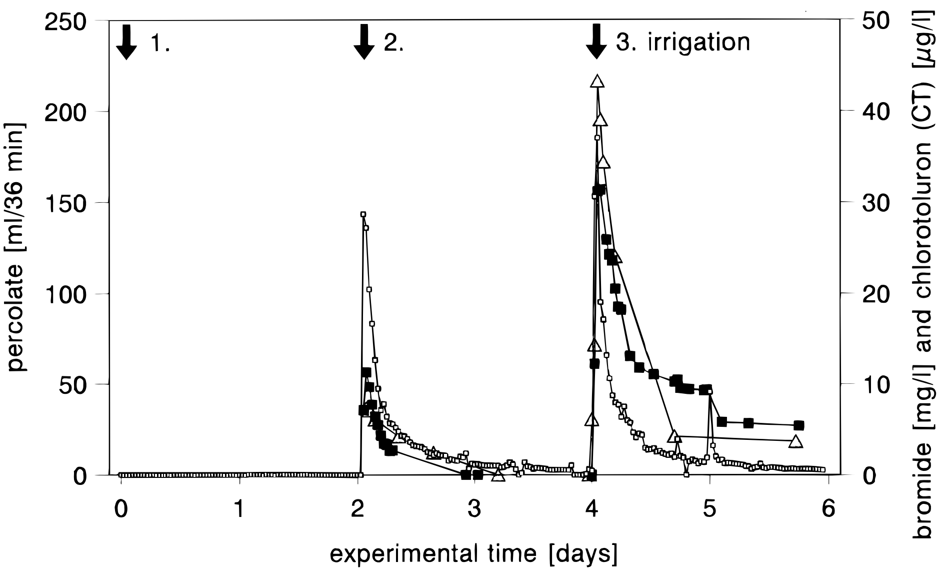

Fig. 3. (□) Percolate and breakthrough curves of (■) bromide and (△) chlorotoluron at the undisturbed soil column S4.

in which a_{ma} is an empirical constant and $\theta_{s\,ma}$ the macropore volume. Water flux into the macropore system (I_{ma}) occurs when the rainfall rate r minus the interception f is larger than the infiltration capacity of the soil matrix (I_{mi}). In this case the soil suction of the upper computational layer n is fixed to an effective maximum soil suction ψ_{eff} and the infiltration rate can be calculated from Darcy's law. According to these assumptions the upper boundary condition of this model is given as

$$\left.\begin{array}{l} I_{mi} = r - f \\ I_{ma} = 0 \end{array}\right\} \psi_n < \psi_{eff}$$

$$\left.\begin{array}{l} I_{mi} = q_{inf\,il} \\ I_{ma} = r - f - q_{inf\,il} \end{array}\right\} \psi_n = \psi_{eff} \tag{5}$$

$$q_{inf\,il} = K(\psi)\left(\frac{\psi_{eff} - \psi_{n-1}}{dz} + 1\right)$$

Only few models consider that $\theta_{s\,ma}$ is not a constant but may vary with soil structural changes due to swelling and shrinking.[16,19] In SIMULAT it is assumed that the soil is rigid.

Solute transport in the soil matrix is computed using the classical convection dispersion equation (CDE)

$$\frac{\partial}{\partial t}(\theta c + \rho s) = \frac{\partial}{\partial z}\left(\theta D_h \frac{\partial c}{\partial z} - qc\right) + Q_s + Q_{ma} \tag{6}$$

in which c is the solute concentration, S the sorbed concentration, ρ the bulk density, and D_h the hydrodynamic dispersion.[20] The term Q_s summarises all sources and sinks of the substances, i.e. all processes creating and consuming the substance and Q_{ma} the exchange term with the macropore system. The solute transport in the macropores as well as the solute exchange between soil matrix and macropores is assumed to be pure convection without any dispersion. Due to the typical flow velocities in macropores, sorption and degradation was neglected in the macropore model. At the upper boundary it was assumed that the concentration of the infiltrating water I_{ma} was in equilibrium with the concentration of the upper computational layer of the soil matrix.

4 EXPERIMENTAL RESULTS

4.1 Visual examination of macropores

In all soil columns S1–S5, a distinctive macropore system was observed (Fig. 2). Clear differences between the columns S1–S5 were found in the topsoil (0–0·30 m). On average, the number of macropores in the subsoil was higher than in the topsoil. From depth 0·45–0·50 m the number of macropores decreased with depth in all columns except column S2. Also in S2 the number decreased from depth 0·6 m to 0·75 m, but the highest quantity was in depth 0·8 and 0·85 m. On average, the number of macropores in the topsoil was 106 pores m^{-2}, in the subsoil 161 pores m^{-2}. Particularly in columns 4 and 5, only few macropores were found in the topsoil. This is a result of soil tillage. By ploughing, macropores are cut off and the soil is mixed in the plough-layer causing a change of water conductivity.[21]

4.2 Herbicide leaching

Figure 3 shows the percolate and the breakthrough curves of bromide and chlorotoluron (CT). There are high concentration peaks of bromide and chlorotoluron after the irrigation. This result is typical for macropore flow.[22] Bromide was detected in columns S2–S5 (Table 4). Because the breakthrough curves are all similar to those for column S4, we decided to show only one column as example. We found CT only in the percolate

TABLE 4
Bromide, Chlorotoluron and Methabenzthiazuron Residues in Percolating Water and Soil Studies Columns S1–S6

Lysimeter	*S1*	*S2*	*S3*	*S4*	*S5*	*S6*
Irrigation water (litres)	3·963	3·963	4·954	4·954	4·954	4·954
Percolate (% of irrigation water)	60·6	66·2	58·2	55·9	71·5	81·9
Bromide in percolate (% of applic. rate)	n.d.	<0·1	4·9	2·4	0·2	n.d.
CT in percolate (% of applic. rate)	n.d.	n.d.	0·1	0·1	n.d.	n.d.
MBT in percolate (% of applic. rate)	n.d.	n.d.	<0·1	n.d.	n.d.	n.d.
Bromide in soil (% of applic. rate)	59·3	64·3	84·3	67·2	79·9	86·9
CT in soil (% of applic. rate)	64·9	64·0	74·4	77·2	78·3	75·2
MBT in soil (% of applic. rate)	74·8	80·6	83·8	85·6	85·8	83·6
Recovery rate (% of application rate)						
Bromide	59·3	64·4	89·2	69·6	71·7	86·9
CT	64·9	64·0	74·5	77·3	78·3	75·2
MBT	74·8	80·6	83·8	85·6	85·8	83·6
Substance share in the topsoil (0–0·30 m) (% of all the substance in the soil)						
Bromide	86·3	76·9	59·6	57·0	68·6	62·1
CT	>99·9	100·0	95·5	98·5	99·9	100·0
MBT	100·0	100·0	98·7	100·0	100·0	100·0
Max. detectable moving depth in soil (m)						
Bromide	0·85	0·85	0·85	0·85	0·85	0·65
CT	0·45	0·25	0·65	0·65	0·45	0·15
MBT	0·25	0·20	0·45	0·20	0·30	0·05

n.d.—not detectable.

of columns S3 and S4, methabenzthiazuron (MBT) only in the percolate of column S3.

Table 4 summarises the results of the soil residue analysis of CT, MBT and bromide for the six lysimeter experiments. The recovery rates for bromide in columns S1, S2, S4 and S5 are rather low. It is possible that, as a result of the high silt and clay content, a part of bromide adsorbed to the soil. The substance share in the topsoil and the maximal detectable moving depth demonstrates the distinction of the water and matter transport in the five undisturbed soil columns S1–S5. However, the difference from the disturbed soil column S6 is marked. Both bromide and herbicide removed deeper into the undisturbed soil columns than into the disturbed soil. To homogenise the samples before herbicide analysis the soil must be dried for two days, so one must consider possible decomposition of CT and MBT when looking at the recovery rate.

5 SIMULATION RESULTS

5.1 Fundamentals

As input parameters, the results of the soil examinations were used as far as possible. The sorption parameters were taken from literature[23,24] (see Table 5). It should be taken into account that these values are not necessarily transferable.

For the calculation of decomposition in SIMULAT, a model is implemented which is described in detail by Richter *et al.*[20] To describe the dependency of degradation on moisture, we applied the non-linear relationship of Richter *et al.*[20] The parameters are given in Table 5.

TABLE 5
Adsorption and Decomposition Parameters of Chlorotoluron (CT) and Methabenzthiazuron (MBT)[a]

	CT	*MBT*	
Ads. parameter topsoil	$K_{oc} = 158{\cdot}7$[23]	$K_{fr} = 6{\cdot}68$[22]	$n = 1{\cdot}47$[22]
Ads. parameter subsoil		$K_{fr} = 1{\cdot}93$[22]	$n = 1{\cdot}27$[22]
k_{opt} (day^{-1})[18]	0·0071	0·011	
θ_{opt} $(cm^3\ cm^{-3})$[18]	0·69	0·553	
a ( )[18]	1·514	2·025	

[a] Sorption function: K_{oc} linear sorption, K_{fr} and n, Freundlich.

Because the temperature was constant in this investigation no temperature dependency was considered. As no data concerning the macropore model were available, macropore parameters were fitted using the experimental results.

First, the water transport in a homogeneous medium was simulated. The nearly homogeneous, packed column, S6, serves as a reference for these simulations. The solute transport was calculated using the water transport and sorption parameters of the herbicides chlorotoluron and methabenzthiazuron obtained from the literature. In the next step, the flow in the undisturbed columns with macropores was simulated. For these calculations, the input data and the knowledge gained from the simulation of the reference column S6 were used. The aim of adding the macropore part to the program was to achieve a good simulation of the measured results in the five undisturbed columns.

5.2 Simulation of the water and solute transport in the packed column S6

Because the soil structure was destroyed, the high intensity of irrigation (3 × 25 mm) resulted in the development of a crust at the soil surface. The water accumulated at the surface. The influence of a surface crust on water transport and the possibility of its simulation are described by Diekkrüger & Bork.[25]

For the packed column, the conductivity and the retention curve of the undisturbed soil samples were used as input data without further calibration. With this parameter vector, the water transport and thus the bromide distribution for the packed column could be well simulated by means of the convection-dispersion equation using the model SIMULAT. The parameter vector well describes the water flow in the soil column and the course of water tension in 25 cm depth, as is shown in Fig. 4. Figure 5 shows the measured and the simulated bromide concentrations for the packed column.

A better agreement could be obtained by using a two-domain model, because the water within the soil aggregates does not take part in the water transport. Hutson & Wagenet[26] developed a multi-region model, a two-domain model extended by considering a region of preferential flow. It is impossible to estimate only with soil characteristic data the distribution of water between the mobile and the immobile phase. Therefore, the partitioning coefficient could be obtained by fitting the model to the bromide data. So far, the model

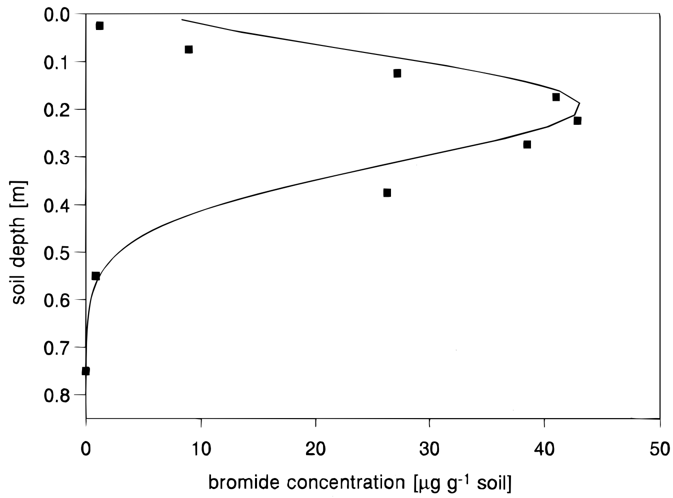

Fig. 5. (■) Measured and (—) simulated bromide movement in the repacked soil column S6 after 75 mm of irrigation. The simulated bromide concentrations refer to the bromide residues found in this column.

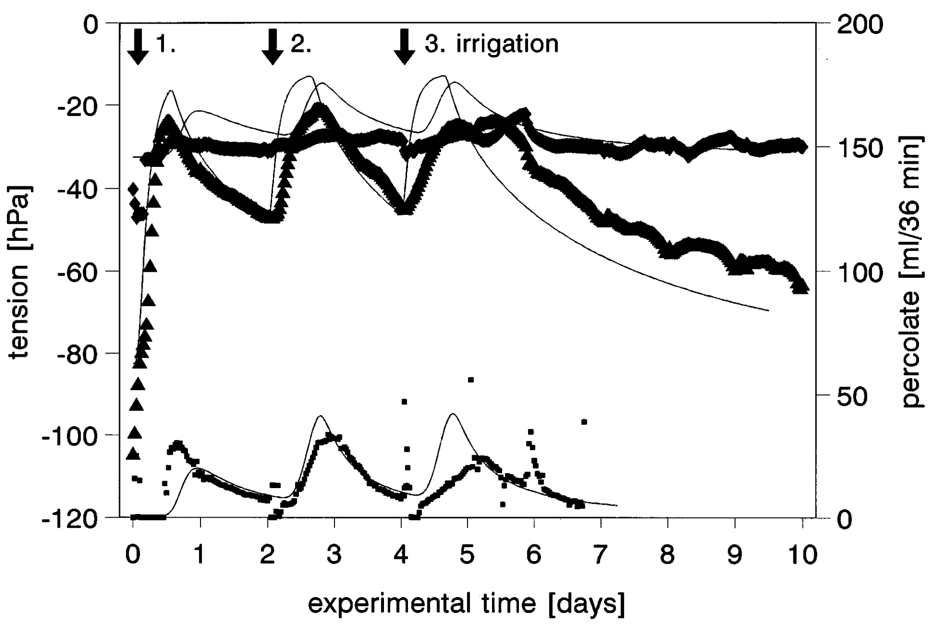

Fig. 4. Simulated and measured water tension at a depth of (▲) 0·25 m and (◆) 0·75 m in the packed column (S6). (—) Simulated and (■) measured temporal course of the percolation rate.

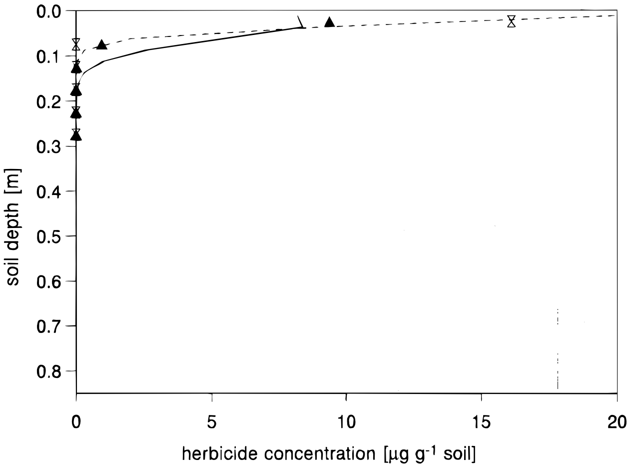

Fig. 6. Simulated and measured (—; ▲) CT and (––; ⧖) MBT concentrations in the repacked soil column S6.

SIMULAT does not consider immobile soil water. For the given soil, the good fit to the measured data suggests that this is not necessary.

With this parameter vector, and the sorption and degradation parameters (Table 5), the transport of CT and MBT was simulated. The result of the simulation is shown in Fig. 6. As for the simulation of the water transport, the parameter vector gives good fits. The different sorption behaviour of the herbicide results in different leaching depths.

5.3 Simulation of water and solute transport in the undisturbed soil

For the input data of the macropore flow ($\theta_{s\,ma}$, $K_{s\,ma}$, a_{ma}, K_{lat}) particular features that were noticed when visually recording the columns, such as the soil crack in column 3 or the smaller number of macropores in the bottom part of the plough horizon, were considered. However, the observed number and size of macropores gave no correlation with the water and solute transport. Therefore, the parameters of macropore flow were obtained by fitting the simulated bromide distribution to the measured distribution. The parameter values of the simulations are shown in Table 6.

For the parameter of the macropore flow model a sensitivity analysis was carried out. It turns out, that the maximum depth of the macropore flow depends on the ratio between the saturated hydraulic conductivity into the macropore system ($K_{s\,ma}$) and the lateral saturated hydraulic conductivity (K_{lat}), the velocity mainly on $K_{s\,ma}$ and the macropore volume ($\theta_{s\,ma}$).

The results of the simulations are shown for column 4 in Figs 7 and 8. As these figures show, the distribution

TABLE 6
Macropore Model Parameters of the Undisturbed Column S4

	Topsoil 1 (0–0·15 m)	*Topsoil 2 (0·15–0·30 m)*	*Subsoil 3 (0·30–0·60 m)*	*Subsoil 2 (0·60–0·85 m)*
$\theta_{s\,ma}$ (cm^3 cm^{-3})	0·2	0·1	0·05	0·01
$K_{s\,ma}$ (cm day^{-1})	160	80	80	10
a_{ma} (–)	1·2	1·2	1·2	1·2
K_{lat} (cm Pa^{-1} day^{-1})	0·3	0·4	0·3	0·3

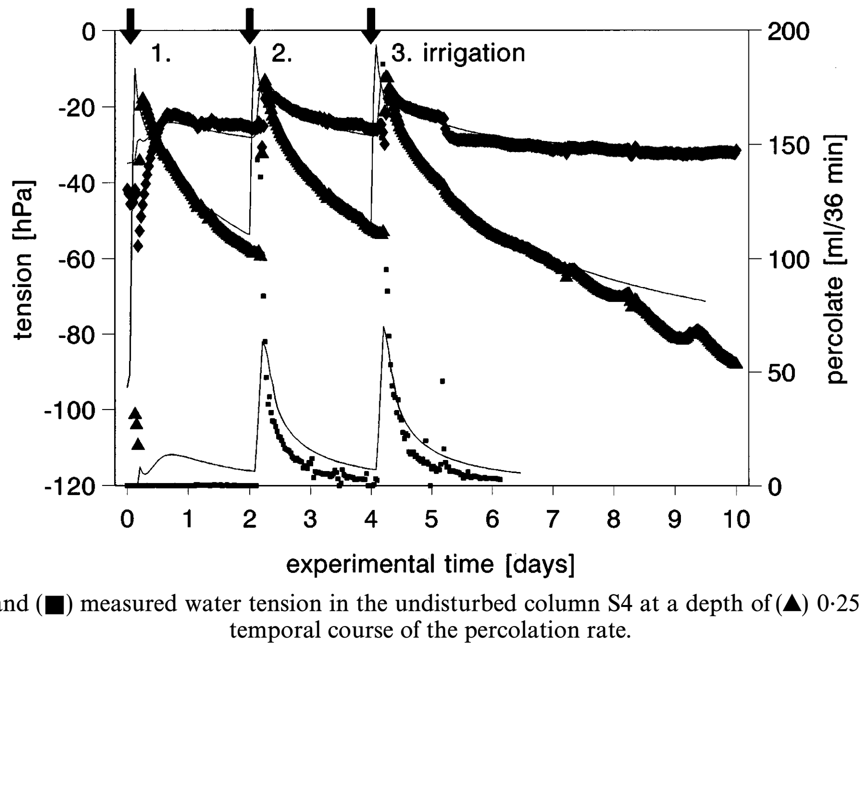

Fig. 7. (—) Simulated and (■) measured water tension in the undisturbed column S4 at a depth of (▲) 0·25 m and (◆) 0·75 m and temporal course of the percolation rate.

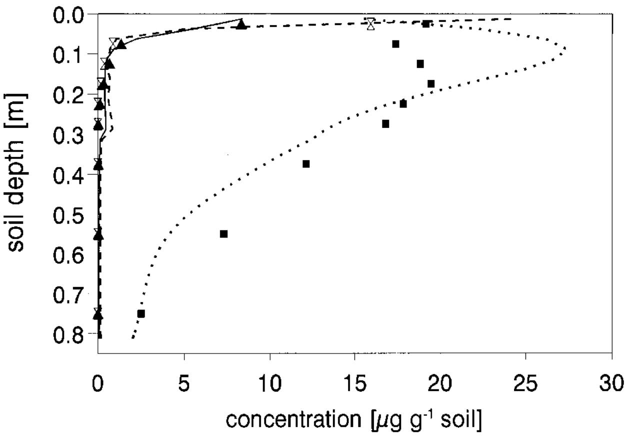

Fig. 8. Comparison of the simulated and measured spatial distribution of (···; ■) bromide, (—; ▲) CT and (--; ⧖) MBT in column S4. The simulated bromide concentrations refer to the bromide residues found in this column.

of bromide, CT and MBT measured in the lysimeter studies could be well simulated using the model SIMULAT. The sudden decrease of the simulated herbicide concentration from topsoil (0–0·30 m) to the subsoil (0·30–0·85 m) can be explained on the basis of the model by different K_d values.

The course of the water retention in the columns at depths of 0·25 m and 0·75 m is also well described by the model. the minor deviations can be explained by small-scale variability. In particular, macropore flow and the resulting lateral infiltration out of the macropores into the soil matrix is significantly influenced by the small-scale spatial variability of soil properties.

6 DISCUSSION

Visual examination showed that none of the five lysimeters had continuous macropores down to the bottom of the soil column. Therefore, the breakthrough curves are the results of lateral infiltration from the macropores into the soil matrix and afterwards leaching through the soil matrix. Because only small amounts of the herbicides were washed out during this experiment, the spatial distribution within the soil column is more important than the breakthrough curves. Because degradation and sorption are significantly reduced below the ploughing layer, a large part of the pesticide crossing this layer may contaminate the groundwater.[27]

The concentration profiles show the continuity of the macropore system is disrupted at ploughing level. This leads to lateral infiltration from the macropores into the soil matrix, resulting in an increased concentration. If saturated conditions exist, the soil water may enter the macropore system again as is illustrated in Fig. 9. How many macropores are active in the subsoil depends on small-scale spatial variability.

The simulation results given in Fig. 8 show that the mean concentration profile is well described, but the typical effect of the ploughing layer is not reproduced.

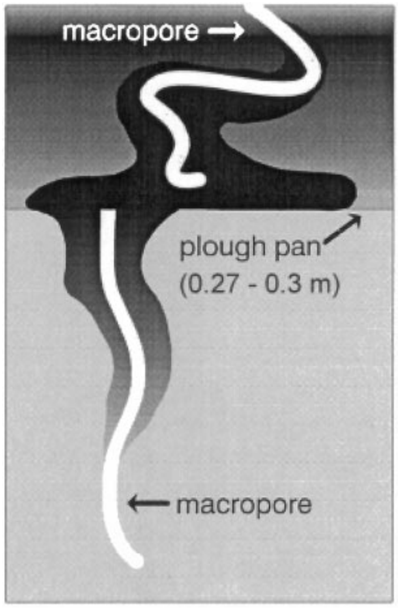

Fig. 9. Proposed water flow in a column at the bottom of the plough horizon.

This is due to the limitations of the model used in this study. The actual version of SIMULAT is able to consider one continuous macropore system. In order to be able to consider the effect of the ploughing layer, it is essential to complete the model system by another independent macropore system and to allow lateral exfiltration and infiltration at the same depth.

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